Table S#. Cartesian coordinates for amide-monoBIP-cyclohexylimine: neutral. (-1169.54988210 Hartrees)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | -0.471013 | 2.719230 | 0.404467 |
| C | -1.870202 | 2.906417 | 0.296027 |
| C | -2.393723 | 4.196481 | 0.184858 |
| C | -1.495704 | 5.264154 | 0.184021 |
| C | -0.111614 | 5.065418 | 0.297463 |
| C | 0.440692 | 3.783150 | 0.418279 |
| C | -1.520203 | 0.761602 | 0.415033 |
| H | -3.461023 | 4.356807 | 0.094799 |
| H | -1.873611 | 6.275398 | 0.091861 |
| H | 0.535348 | 5.934541 | 0.275421 |
| N | -2.493061 | 1.668373 | 0.309223 |
| C | -3.064558 | -1.180883 | 0.359005 |
| C | -1.740478 | -0.674759 | 0.437918 |
| C | -0.656527 | -1.560914 | 0.512119 |
| C | -0.842709 | -2.937533 | 0.512881 |
| C | -2.162572 | -3.407603 | 0.441611 |
| C | -3.284265 | -2.577537 | 0.367178 |
| H | 0.349407 | -1.160354 | 0.564120 |
| H | -2.324358 | -4.474191 | 0.443043 |
| C | 0.372067 | -3.870485 | 0.562377 |
| C | -4.703466 | -3.164133 | 0.294389 |
| O | -4.120509 | -0.340363 | 0.274156 |
| H | -3.773508 | 0.597669 | 0.268360 |
| N | -0.287037 | 1.359615 | 0.480757 |
| H | 0.631217 | 0.939665 | 0.537028 |
| C | 1.888924 | 3.472959 | 0.551452 |
| C | 1.236211 | -3.630258 | -0.692437 |
| H | 1.560530 | -2.588531 | -0.751958 |
| H | 2.128127 | -4.263454 | -0.667599 |
| H | 0.676152 | -3.864086 | -1.601848 |
| C | 1.212889 | -3.557266 | 1.815795 |
| H | 0.634486 | -3.729862 | 2.727402 |
| H | 2.098218 | -4.199146 | 1.845727 |
| H | 1.550258 | -2.517789 | 1.818098 |
| C | -0.032944 | -5.350114 | 0.602283 |
| H | -0.630636 | -5.581040 | 1.488274 |
| H | -0.607251 | -5.635205 | -0.283545 |
| H | 0.864667 | -5.972723 | 0.632625 |
| C | -5.382271 | -2.736305 | -1.023974 |
| H | -6.394280 | -3.149723 | -1.070858 |
| H | -5.446118 | -1.652031 | -1.105040 |
| H | -4.821026 | -3.115547 | -1.882644 |
| C | -5.536110 | -2.677154 | 1.499787 |
| H | -5.637656 | -1.592723 | 1.500692 |
| H | -6.535677 | -3.120853 | 1.465186 |
| H | -5.061653 | -2.980695 | 2.437132 |
| C | -4.687461 | -4.701279 | 0.330629 |
| H | -4.135209 | -5.121203 | -0.514251 |
| H | -4.241050 | -5.081316 | 1.253410 |
| H | -5.714901 | -5.069031 | 0.276888 |
| O | 2.289504 | 2.296552 | 0.528805 |
| N | 2.746838 | 4.509291 | 0.681735 |
| H | 2.432542 | 5.446434 | 0.872382 |
| H | 3.716352 | 4.293268 | 0.856797 |

Table S#. Cartesian coordinates for amide-monoBIP-cyclohexylimine: E0PT. (-1169.35039383 Hartrees)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | -0.460429 | 2.735524 | 0.446323 |
| C | -1.869382 | 2.860977 | 0.319118 |
| C | -2.459229 | 4.128065 | 0.212125 |
| C | -1.611824 | 5.226396 | 0.239777 |
| C | -0.212951 | 5.087825 | 0.366657 |
| C | 0.403475 | 3.841091 | 0.470839 |
| C | -1.402163 | 0.736962 | 0.439368 |
| H | -3.531181 | 4.239010 | 0.111285 |
| H | -2.027979 | 6.223212 | 0.162848 |
| H | 0.385151 | 5.990745 | 0.386241 |
| N | -2.418292 | 1.600557 | 0.320075 |
| C | -2.981818 | -1.178361 | 0.350491 |
| C | -1.610148 | -0.691346 | 0.456400 |
| C | -0.575082 | -1.600797 | 0.544414 |
| C | -0.825097 | -2.986204 | 0.536308 |
| C | -2.167945 | -3.436468 | 0.442228 |
| C | -3.256643 | -2.596661 | 0.352899 |
| H | 0.445286 | -1.247657 | 0.614561 |
| H | -2.340147 | -4.499892 | 0.440207 |
| C | 0.344584 | -3.953435 | 0.600540 |
| C | -4.687489 | -3.124153 | 0.253743 |
| O | -3.964111 | -0.334742 | 0.243709 |
| H | -3.574839 | 0.649737 | 0.249351 |
| N | -0.206714 | 1.390931 | 0.521192 |
| H | 0.737656 | 1.034509 | 0.618380 |
| C | 1.868559 | 3.589189 | 0.592765 |
| C | 1.231363 | -3.712792 | -0.644456 |
| H | 1.598602 | -2.685387 | -0.680988 |
| H | 2.093341 | -4.383355 | -0.604857 |
| H | 0.677092 | -3.916211 | -1.563499 |
| C | 1.171921 | -3.665528 | 1.874069 |
| H | 0.573104 | -3.825687 | 2.773318 |
| H | 2.026535 | -4.345768 | 1.903068 |
| H | 1.553789 | -2.642931 | 1.888956 |
| C | -0.099791 | -5.421726 | 0.620714 |
| H | -0.717561 | -5.645628 | 1.494086 |
| H | -0.657753 | -5.688837 | -0.280284 |
| H | 0.785206 | -6.059173 | 0.665662 |
| C | -5.318263 | -2.681336 | -1.086270 |
| H | -6.327499 | -3.094501 | -1.155508 |
| H | -5.385280 | -1.597440 | -1.168956 |
| H | -4.736228 | -3.061420 | -1.929323 |
| C | -5.525635 | -2.591310 | 1.438599 |
| H | -5.615198 | -1.506346 | 1.416330 |
| H | -6.528499 | -3.022147 | 1.386748 |
| H | -5.075468 | -2.885194 | 2.389897 |
| C | -4.714164 | -4.660198 | 0.305642 |
| H | -4.159200 | -5.104099 | -0.524841 |
| H | -4.298834 | -5.039954 | 1.242534 |
| H | -5.750160 | -4.996818 | 0.235438 |
| O | 2.292593 | 2.425831 | 0.702111 |
| N | 2.693045 | 4.653346 | 0.587151 |
| H | 2.374103 | 5.593269 | 0.419829 |
| H | 3.687634 | 4.487257 | 0.620327 |

Table S#. Cartesian coordinates for amide-monoBIP-cyclohexylimine: E1PT. (-1169.36621356 Hartrees)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | -0.484912 | 2.742772 | 0.431986 |
| C | -1.873615 | 2.958505 | 0.377560 |
| C | -2.407400 | 4.244916 | 0.313207 |
| C | -1.494219 | 5.295135 | 0.310520 |
| C | -0.105210 | 5.077738 | 0.365757 |
| C | 0.440471 | 3.794168 | 0.426227 |
| C | -1.494794 | 0.753089 | 0.449032 |
| H | -3.474761 | 4.413493 | 0.265328 |
| H | -1.861289 | 6.312502 | 0.262797 |
| H | 0.545778 | 5.943262 | 0.358718 |
| N | -2.450222 | 1.700633 | 0.391313 |
| C | -3.104629 | -1.173812 | 0.357770 |
| C | -1.725783 | -0.672873 | 0.464089 |
| C | -0.665956 | -1.549334 | 0.558846 |
| C | -0.865644 | -2.947302 | 0.549275 |
| C | -2.183024 | -3.438874 | 0.440318 |
| C | -3.299036 | -2.628504 | 0.344932 |
| H | 0.345933 | -1.173525 | 0.643605 |
| H | -2.322353 | -4.508179 | 0.430390 |
| C | 0.348050 | -3.861854 | 0.631814 |
| C | -4.706659 | -3.204895 | 0.227827 |
| O | -4.068744 | -0.371888 | 0.277269 |
| N | -0.297941 | 1.377500 | 0.476550 |
| H | 0.637868 | 0.982793 | 0.501224 |
| C | 1.892365 | 3.449439 | 0.467721 |
| C | 1.249708 | -3.576758 | -0.591131 |
| H | 1.571246 | -2.533177 | -0.615556 |
| H | 2.141524 | -4.206507 | -0.540391 |
| H | 0.723394 | -3.798850 | -1.522615 |
| C | 1.133478 | -3.548135 | 1.924328 |
| H | 0.522163 | -3.738580 | 2.809199 |
| H | 2.015964 | -4.190695 | 1.971533 |
| H | 1.471129 | -2.509821 | 1.954257 |
| C | -0.033123 | -5.347717 | 0.634362 |
| H | -0.652697 | -5.604809 | 1.497423 |
| H | -0.569567 | -5.627956 | -0.275591 |
| H | 0.876564 | -5.949484 | 0.684424 |
| C | -5.342845 | -2.753034 | -1.106920 |
| H | -6.347552 | -3.176435 | -1.185453 |
| H | -5.415974 | -1.668339 | -1.167626 |
| H | -4.755234 | -3.114080 | -1.955050 |
| C | -5.567222 | -2.714196 | 1.414945 |
| H | -5.677713 | -1.631497 | 1.398964 |
| H | -6.558433 | -3.171339 | 1.354851 |
| H | -5.112694 | -3.005752 | 2.365393 |
| C | -4.693771 | -4.741435 | 0.250824 |
| H | -4.121201 | -5.155633 | -0.583038 |
| H | -4.276886 | -5.129740 | 1.183614 |
| H | -5.720329 | -5.103372 | 0.165284 |
| O | 2.245992 | 2.257998 | 0.501391 |
| N | 2.775117 | 4.462561 | 0.467213 |
| H | 2.500896 | 5.430215 | 0.421799 |
| H | 3.759522 | 4.243189 | 0.480774 |
| H | -3.430014 | 1.422387 | 0.352680 |

Table S#. Cartesian coordinates for amide-monoBIP-cyclohexylimine: E2PT. (-1169.35567448 Hartrees)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | -0.527014 | 2.714588 | 0.427516 |
| C | -1.909055 | 2.974525 | 0.291997 |
| C | -2.394626 | 4.274071 | 0.180270 |
| C | -1.453489 | 5.308416 | 0.206050 |
| C | -0.079948 | 5.067957 | 0.344054 |
| C | 0.414124 | 3.761689 | 0.462404 |
| C | -1.505324 | 0.789626 | 0.416936 |
| H | -3.452029 | 4.478784 | 0.071821 |
| H | -1.796353 | 6.331300 | 0.117990 |
| H | 0.594180 | 5.915516 | 0.355087 |
| N | -2.490361 | 1.726673 | 0.292805 |
| C | -3.119246 | -1.161314 | 0.336256 |
| C | -1.748567 | -0.640870 | 0.433854 |
| C | -0.677667 | -1.505850 | 0.521103 |
| C | -0.858727 | -2.903849 | 0.524037 |
| C | -2.173186 | -3.414399 | 0.443508 |
| C | -3.298416 | -2.618375 | 0.354005 |
| H | 0.322045 | -1.094590 | 0.580987 |
| H | -2.298893 | -4.485612 | 0.451438 |
| C | 0.366826 | -3.805547 | 0.590679 |
| C | -4.702515 | -3.213817 | 0.274013 |
| O | -4.096245 | -0.373870 | 0.237528 |
| N | -0.296396 | 1.366735 | 0.503430 |
| C | 1.814594 | 3.395675 | 0.621095 |
| C | 1.248233 | -3.515747 | -0.645225 |
| H | 1.553213 | -2.467599 | -0.679165 |
| H | 2.149838 | -4.132485 | -0.604236 |
| H | 0.713217 | -3.749581 | -1.568936 |
| C | 1.168231 | -3.477392 | 1.869023 |
| H | 0.576762 | -3.679859 | 2.764990 |
| H | 2.065985 | -4.099936 | 1.902576 |
| H | 1.481018 | -2.431276 | 1.891175 |
| C | 0.004137 | -5.296029 | 0.602903 |
| H | -0.598207 | -5.558767 | 1.476421 |
| H | -0.544674 | -5.584532 | -0.297177 |
| H | 0.921353 | -5.887654 | 0.638954 |
| C | -5.368251 | -2.804110 | -1.059228 |
| H | -6.367788 | -3.244277 | -1.112485 |
| H | -5.458700 | -1.722329 | -1.142961 |
| H | -4.788652 | -3.174730 | -1.908879 |
| C | -5.549864 | -2.706825 | 1.463678 |
| H | -5.660407 | -1.624206 | 1.434827 |
| H | -6.542340 | -3.163781 | 1.422880 |
| H | -5.084500 | -2.986786 | 2.412439 |
| C | -4.670899 | -4.749397 | 0.334707 |
| H | -4.109725 | -5.177305 | -0.500123 |
| H | -4.227618 | -5.107421 | 1.267530 |
| H | -5.694261 | -5.126489 | 0.280422 |
| O | 2.152359 | 2.137227 | 0.689980 |
| N | 2.789425 | 4.270832 | 0.708043 |
| H | 2.622135 | 5.265214 | 0.684808 |
| H | 3.741021 | 3.946652 | 0.815779 |
| H | -3.465489 | 1.449139 | 0.218568 |
| H | 1.324753 | 1.545401 | 0.629920 |